

Gluconolactone
90-80-2 | DTXSID0026549

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 314 °C

Global applicability domain: Outside

Local applicability domain index: 1.80e-01

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Erythritol</div> <div>Measured: 331</div> <div>Predicted: 327</div>	<div>Image not found</div> <div>Pyrogallol</div> <div>Measured: 309</div> <div>Predicted: 292</div>	<div>Image not found</div> <div>Triisopropanolamine</div> <div>Measured: 305</div> <div>Predicted: 302</div>
<div>Image not found</div> <div>2-(Hydroxymethyl)-2-methyl-1,3-propanediol</div> <div>Measured: 283</div> <div>Predicted: 289</div>	<div>Image not found</div> <div>Triethanolamine</div> <div>Measured: 335</div> <div>Predicted: 326</div>	